Coulomb interaction at the metal-insulator critical point in graphene

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We compute the renormalization group flow of the long-ranged electron-electron interaction at the Gross-Neveu quantum critical point between the semimetal and the excitonic insulator in graphene, perturbatively in the small parameter $\epsilon = d-1$, with d as the spatial dimension. The $O(\epsilon)$ correction to the usual beta-function makes the long-range interaction only more irrelevant at the critical than at the Gaussian fixed point. A weak long-range tail of the Coulomb interaction is found to be marginally irrelevant also in arbitrary dimension when the number of Dirac fermions is large. Its ultimate irrelevancy notwithstanding, it is shown that the metal-insulator transition may still be induced by increasing only the long-range tail of the Coulomb interaction.

Increasing the strength of electron-electron interactions relative to the bandwidth is expected to transform graphene from its usual semi-metallic phase into the gapped Mott insulator. This quantum phase transition has been studied by a variety of numerical [1, 2, 3, 4] and analytical [5, 6, 7, 8, 9] techniques, and it represents a condensed matter analog of the particle physics phenomenon of chiral symmetry breaking. Graphene provides 2+1-dimensional Dirac fermions [10] where the presence of two valleys and two spin states result in $SU(4)$ chiral symmetry, which can be broken to $SU(2) \times SU(2)$ while still preserving parity and time reversal invariance. Similar systems have been studied [11]-[13] as toy models of strong coupling behavior in quantum chromodynamics and technicolor theories. In graphene, this results in breaking of the sublattice symmetry and gapping the electron spectrum. Generation and control of such a gap is of great importance to potential applications in electronics [14].

One issue of contention is the precise role in the mechanism of the transition of the long-ranged $\sim 1/r$ tail of Coulomb interaction, which remains unscreened when graphene is at the Dirac point. Whereas the initial analytical calculations based on the Schwinger-Dyson equations [5, 6] found that the long-range interaction is crucial and leads to an essential singularity in the free energy, recent numerical calculations [4] find only a regular second-order transition. The analytic expansion around the exactly solvable three-dimensional limit of the theory [9, 13] also yields a regular critical point at which a weak long-range interaction may be shown to represent a marginally irrelevant perturbation. In the present study we complement these results by showing that a weak unscreened $\sim 1/r$ tail of the electron-electron repulsion remains a marginally irrelevant perturbation for an arbitrary number of Dirac fermion components N at the metal-insulator quantum critical point near one spatial dimension, as well as for large N in arbitrary spatial dimension. This is accomplished by computing the *first correction* to the beta-function of the long-range coupling constant, which we shall henceforth call the *charge*. This correction is $O(\epsilon)$ relative to the leading term, with $\epsilon = d-1$, and its sign is such that the flow of the charge towards zero, although logarithmic in either case, becomes *faster* at the quantum critical than at the Gaussian fixed point (Fig. 1). The renormalization-group flow also implies that the transition may be tuned by the charge alone, and can then occur even at a sub-critical value of the short-range interaction.

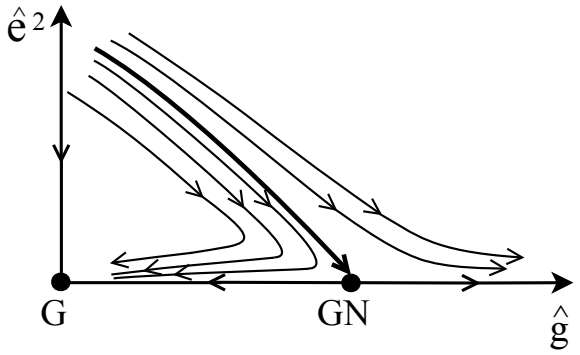

FIG. 1: Schematic renormalization-group flow in the infrared for the metal-insulator transition in graphene. $\hat{g}$ is the (dimensionless) short-range, and $\hat{e}^2$ the long-range component of the Coulomb electron-electron interaction. GN and G are the critical Gross-Neveu and the Gausian fixed points, respectively.

We consider the simplest Gross-Neveu Lagrangian that should suffice to describe the quantum phase transition into the gapped excitonic (charge-density-wave) phase with increase of nearest-neighbor repulsion in graphene, tuned to be at the Dirac point [7, 8],

$$L = \bar{\Psi}_\alpha \gamma_0 (\partial_0 + ia)\Psi_\alpha + v\bar{\Psi}_\alpha \gamma_i \partial_i \Psi_\alpha \qquad (1)$$
$$-g(\bar{\Psi}_\alpha \Psi_\alpha)^2 + \frac{1}{2e_d^2} a|\nabla|^{d-1} a.$$

The short-range coupling $g > 0$ is proportional to the nearest-neighbor repulsive interaction [7], and the four-component Dirac fermion Ψ_α is defined using the conventions of [7, 8]. For generality we will assume an arbitrary number of Dirac fermions N, so $\alpha = 1, 2, ...N$. For physical spin-1/2 electrons $N = 2$. The Dirac matrices

satisfy the standard Clifford algebra in Euclidian spacetime $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$. For simplicity, we do not consider the transition to a spin-density wave phase [7, 9]. Our calculation can easily be modified to consider that case as well and the conclusion would be similar.

Integration over the gauge field a introduces the instantaneous density-density long-range interaction

$$\bar{\Psi}_\alpha \gamma_0 \Psi_\alpha(\vec{x},\tau) \frac{e^2}{2|\vec{x}-\vec{y}|} \bar{\Psi}_\alpha \gamma_0 \Psi_\alpha(\vec{y},\tau), \tag{2}$$

in any spatial dimension d, provided that we define

$$e_d^2 = e^2 (4\pi)^{\epsilon/2} \Gamma(\epsilon/2), \tag{3}$$

and $\epsilon = d-1$. Note that as $\epsilon \to 0$ the coupling e_d defined this way diverges. This reflects the fact that the Fourier transform of $\sim 1/r$ interaction in $d = 1$ is $\sim \ln(k)$ [15]. We will confine out attention to the region $d > 1$ in the following.

Let us first outline our method and principal result. Since the inverse of the gauge-field propagator is a non-analytic function of the momenta for dimensions $1 < d < 2$, the coupling e_d cannot renormalize [16], and

$$\frac{de^2}{d\ln\Lambda} = 0, \tag{4}$$

where Λ is the ultraviolet cutoff. The instantaneous long-range interaction does not respect the Lorentz invariance, however, and consequently renormalizes the Fermi velocity. At a momentum scale $k \ll \Lambda$ one expects the velocity to become

$$v(k) = v + a_d e_d^2 \ln(\frac{\Lambda}{k}) + b_d e_d^2 \hat{g} [\ln(\frac{\Lambda}{k})]^n + O(\frac{e_d^4}{v}, e_d^2 \hat{g}^2), \tag{5}$$

where a_d and b_d are d-dependent numerical coefficients, and $\hat{g} = g\Lambda^\epsilon/\pi$ is the *dimensionless* short-range coupling. The coefficient a_d for $d = 2$ has been computed earlier [7, 17, 18, 19]. Since $v(k)$ is a physical observable it must be independent of the arbitrary cutoff Λ, i. e.

$$\frac{dv(k)}{d\Lambda} = 0, \tag{6}$$

at *all* momenta k. This condition of renormalizability of the field theory in Eq. (1) can be satisfied only if the power of the logarithm in the third term in Eq. (5) is $n = 1$, and if $d\hat{g}/d\Lambda = 0$. Since the beta-function for the Gross-Neveu coupling, as it will be shown later, reads

$$\frac{d\hat{g}}{d\ln\Lambda} = \epsilon\hat{g} + (1 - \frac{2}{\epsilon})\hat{g}\hat{e}^2 - 2(2N-1)\hat{g}^2 + O(\hat{g}^2\hat{e}^2, \hat{g}^3), \tag{7}$$

where $\hat{e}^2 = e^2/\pi v$ is the *dimensionless charge* which measures the strength of the long-range coupling relative to the Fermi velocity, the condition of renormalizability at $\hat{e}^2 = 0$ is satisfied only at the fixed points: 1) Gaussian, $\hat{g}_G = 0$, and 2) the critical $\hat{g}_c = \epsilon/(2(2N-1)) + O(\epsilon^2)$. Eqs. (5) and (6) yield then the beta-function for the Fermi velocity

$$\frac{dv}{d\ln\Lambda} = -e_d^2 (a_d + b_d \hat{g}^*). \tag{8}$$

$\hat{g}^*$ is one of the above two fixed points. We can then recast Eqs. (4) and (8) together as the equation for the dimensionless charge

$$\frac{d\hat{e}^2}{d\ln\Lambda} = \hat{e}^4 \pi (4\pi)^{\epsilon/2} \Gamma(\epsilon/2)(a_d + b_d \hat{g}^*). \tag{9}$$

Both of the coefficients a_d and b_d turn out to be $O(\epsilon)$. Therefore the divergent $\sim 1/\epsilon$ prefactor in the last equation cancels. We thus find a regular expansion of the beta-function for the dimensionless charge in powers of ϵ and $\hat{e}^2$,

$$\frac{d\hat{e}^2}{d\ln\Lambda} = \hat{e}^4 \left(1 + \frac{\epsilon}{2(2N-1)} + O(\epsilon^2/N)\right) + O(\hat{e}^6). \tag{10}$$

There are two notable features of the last expression. First, the $O(\epsilon)$ correction has the same sign as the leading term. As a result, the long-range interaction is in fact more irrelevant in the infrared, although still marginally so, than at the Gaussian fixed point. Second, the correction is $O(1/N)$. Therefore, for a large number of Dirac fermions, the Coulomb interaction is also marginally irrelevant in all dimensions. Together with the previous analysis near three spatial dimensions [9] this means that a weak long-range tail of Coulomb interaction is an irrelevant perturbation at the Gross-Neveu metal-insulator quantum critical point in *all* perturbatively accessible regimes of the theory.

The beta-function for the short-range coupling in Eq. (7), besides the usual terms [7, 8] obtains the contribution from the long-range Coulomb interaction. The sign of this term is *negative*, so that there is a trajectory in the region $\hat{g} < \hat{g}_c$ that flows right into the critical point and separates the flows towards the semimetallic and the insulating ground states, as depicted in Fig. 1. The negative sign is crucial to this result, which we may have expected on physical grounds: that an increase of the charge alone should take the semimetal towards the insulator. This situation may be analogous to the one in $3+1$-dimensional quantum electrodynamics, where the chiral-symmetry-breaking transition may also be tuned by the electromagnetic charge, but the critical behavior seems, on the other hand, to be controlled by the Nambu-Jona-Lasinio theory with only short-range interactions [20, 21].

Let us now present the calculational details. The logarithmic terms in Eq. (5) derive from the diagrams in Figs. (2)-(3). Diagrams in Fig. (3), however, do not contribute to the renormalization of the Fermi velocity. Since the fixed-point interaction is a contact interaction, the diagram in Fig. (3b) vanishes, whereas the diagram in Fig. (3c) is independent of the external momentum. The diagram in Fig. (3a), which is also the only diagram to this order which would be of order N, vanishes

FIG. 2: One- and two-loop diagrams that renormalize the Fermi velocity. The wavy line is the long-range interaction, and the dashed line is the contact fixed-point interaction.

as well because it is proportional to the factor $Tr\gamma_0 = 0$ that accompanies the fermion loop. This implies that both the coefficients a_d and b_d as far as the number of Dirac fermions N is concerned are $O(1)$. Since the fixed point interaction is $\hat{g}_c \sim 1/N$, it guarantees that the first correction to the Gaussian result is also $O(1/N)$.

One is therefore left with the diagrams in Fig. (2) to compute. Defining the self-energy from the Dirac fermion propagator $G(k)$ as

$$G^{-1}(k) = ik_0\gamma_0 + ivk_i\gamma_i + \Sigma(k), \tag{11}$$

where the $d+1$-momentum $k = (k_0, \vec{k})$, we can write both contributions together as

$$\Sigma(k) = ie_d^2 \int \frac{dq}{(2\pi)^{d+1}} \frac{q_\alpha + k_\alpha}{|\vec{q}|^\epsilon (q+k)^2} \{-\gamma_0\gamma_\alpha\gamma_0 + 2g(\gamma_\mu\gamma_0\gamma_\nu\gamma_\alpha\gamma_0 + \gamma_0\gamma_\alpha\gamma_\nu\gamma_0\gamma_\mu) I_{\mu\nu}(q)\}, \tag{12}$$

where $dq = dq_0 d^d\vec{q}$, and the integral

$$I_{\mu\nu}(q) = \int \frac{dp}{(2\pi)^{d+1}} \frac{p_\mu (p+q)_\nu}{p^2 (p+q)^2}. \tag{13}$$

We have set the Fermi velocity in the last two equations to $v = 1$ for notational simplicity. Since the integral over the momentum q in the first term is only logarithmically divergent in the infrared, for the divergent part of the self-energy we need to include only the $q = 0$ limit of $I_{\mu\nu}(q)$. In any $d > 1$ the integral $I_{\mu\nu}(q)$ is infrared convergent and may be easily computed to be

$$I_{\mu\nu}(q) = \frac{\Lambda^\epsilon \delta_{\mu\nu}}{4\pi\epsilon} + O(q^\epsilon) \tag{14}$$

when $\epsilon \ll 1$. On the other hand,

$$\delta_{\mu\nu}(\gamma_\mu\gamma_0\gamma_\nu\gamma_\alpha\gamma_0 + \gamma_0\gamma_\alpha\gamma_\nu\gamma_0\gamma_\mu) = 2(1-d)\gamma_0\gamma_\alpha\gamma_0, \tag{15}$$

where we analytically continued the identity $\gamma_i\gamma_i = d$ to arbitrary spatial dimension d. The self-energy therefore simplifies into

$$\Sigma(k) = -ie_d^2\gamma_0\gamma_\alpha\gamma_0 (1 + \frac{g\Lambda^\epsilon}{\pi}) \int \frac{dq}{(2\pi)^{d+1}} \frac{q_\alpha + k_\alpha}{|\vec{q}|^\epsilon (q+k)^2}, \tag{16}$$

and becomes simply proportional to the leading contribution. The remaining integral may be performed in arbitrary dimension $d > 1$, and it yields

$$\Sigma(k) = \frac{(1-d^{-1})e_d^2}{\Gamma(d/2) 2^d \pi^{d/2}} (1 + \frac{g\Lambda^\epsilon}{\pi}) \ln(\frac{\Lambda}{k}) ik_i\gamma_i. \tag{17}$$

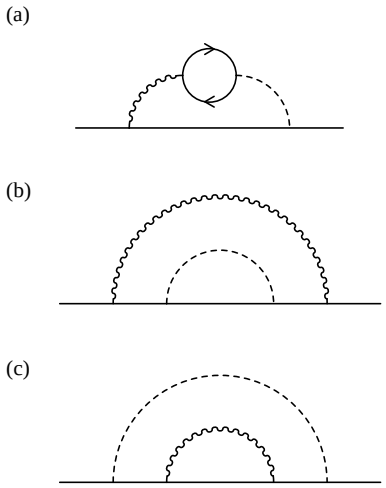

FIG. 3: The remaining three two-loop diagrams that do not contribute to the Fermi velocity renormalization.

In the limit $d \to 1$ the diverging part of the self-energy therefore becomes

$$\Sigma(k) = \frac{e^2}{\pi}(1+\hat{g}) \ln(\frac{\Lambda}{k}) ik_i\gamma_i. \tag{18}$$

Replacing the Gross-Neveu coupling $\hat{g}$ with its $O(\epsilon)$ critical value the last result may be recast as in Eq. (10).

We turn now to the calculation of the beta-function of the short-range coupling in presence of the long-range Coulomb interaction. Since the Coulomb coupling violates effective Lorentz invariance of the Gross-Neveu Lagrangian, the engineering dimension of the short-range coupling constant receives an additional contribution from a non-trivial dynamical exponent z, and it is equal to $\epsilon - (z-1)$. The beta-function of the short-range coupling then becomes

$$\frac{d\hat{g}}{d\ln\Lambda} = (\epsilon - z + 1)\hat{g} - 2(2N-1)\hat{g}^2 + c_d\hat{e}^2\hat{g} + O(\hat{g}^2\hat{e}^2, \hat{g}^3), \tag{19}$$

where the third term arises from the diagrams shown in Fig. 4, and the term proportional to $\hat{g}^2$ yields the usual beta-function for the Gross-Neveu coupling in the absence of other interactions [7, 8]. In fact, only the diagram in Fig. 4a renormalizes the short-range coupling, $g \to g + \delta g$, where

$$\delta g = -\frac{4\pi}{\epsilon}\hat{e}^2 g \int \frac{dq}{(2\pi)^{d+1}} \frac{1}{(q+k)^2 |\vec{q}|^\epsilon}. \tag{20}$$

This integral may be performed in arbitrary dimension $d > 1$, similarly to the one in Eq. (17), and in the limit $d \to 1$ its diverging part has the form

$$\delta g = -\frac{2}{\epsilon}\hat{e}^2 g \ln(\frac{\Lambda}{k}), \tag{21}$$

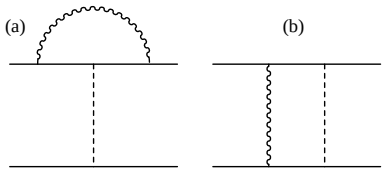

FIG. 4: Renormalization of the Gross-Neveu coupling due to the long-range Coulomb interaction.

yielding $c_d = -2/\epsilon$ in Eq. (19). The remaining diagram in Fig. 4b does not renormalize the Gross-Neveu coupling, but generates a new short-range coupling of the form $(\bar{\Psi}\gamma_0\vec{\gamma}\Psi)^2$, which is irrelevant close to the critical point. An analogous situation arises in the $(2+1)$-dimensional quantum electrodynamics with the additional Gross-Neveu interaction [22]. The irrelevance of the generated short-range interaction also agrees with the emergent Lorentz invariance in graphene [8]. Finally, identifying the right-hand side of Eq. (8) as being precisely $(z-1)e_d^2$ [7] yields the beta-function of the Gross-Neveu coupling as in Eq. (7).

Remarkably, it is possible to obtain the explicit solution of the flow-equations in Eqs. (7) and (10). Since the long-range Coulomb interaction is marginally irrelevant in the infrared, it is convenient to cast the two flow equations in the form

$$e^4 dg/de^2 = \epsilon g - 2(2N-1)g^2 - (2/\epsilon - 1)ge^2, \qquad (22)$$

where we dropped the hats on the dimensionless couplings, and neglected the term $\sim \epsilon$ in Eq. (10). General solution of this differential equation reads

$$g(e^2) = g_c \frac{(\epsilon/e^2)^{(2/\epsilon-1)} \mathrm{e}^{-\epsilon/e^2}}{C + \Gamma(2/\epsilon, \epsilon/e^2)}, \qquad (23)$$

with C as the integration constant, $\Gamma(a,b) \equiv \int_b^\infty t^{a-1}\mathrm{e}^{-t}dt$. Depending on the initial condition, Eq. (23) describes the infrared flow of the short-range coupling towards either zero or infinity. The trajectory ending exactly at the critical point as the charge flows to zero, $g(e^2 \to 0) = g_c$, separates two regions with different asymptotic behavior of the flow in the infrared, as in Fig. 1. The separatrix is obtained by setting $C = 0$ in Eq. (23), so that the solution near the Gross-Neveu critical point becomes

$$\frac{g(e^2)}{g_c} = 1 - \frac{2-\epsilon}{\epsilon^2} e^2 + O(e^4). \qquad (24)$$

The separatrix therefore lies in the region $g < g_c$, and approaches the critical value of the Gross-Neveu coupling as the charge flows to zero *linearly*.

To summarize, we have computed the beta-function governing the flow of the long-range tail of the Coulomb interaction at the Gross-Neveu metal-insulator quantum critical point in an expansion near one spatial dimension. The effect of the short-range Gross-Neveu interaction is to render the charge more (marginally) irrelevant than at the Gaussian fixed point. We discussed how the form of the flow diagram implies that the (irrelevant) charge is nevertheless a possible tuning parameter for the metal-insulator transition in graphene.

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